Approach to a Uniform Theory of the Liquid and Solid Phases of \(^4\)He at Absolute Zero

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(Received December 27, 1973)

Theoretical studies of liquid \(^4\)He have led to recognition of a plausible general form for the exact ground-state wave function. Arguments are presented supporting the view that the same form is adequate to describe the solid. The notion of a local density is used to adapt the form to the description of the two-phase density range. Van Hove’s theorem holds for the ground state.

A crystalline solid is usually described in terms of fixed symmetry axes and fixed lattice sites with respect to the laboratory reference frame.\(^1\) Let \(\psi_s\) denote the ground-state wave function under the stated conditions. An alternative description which does not specify the orientation of the symmetry axes and the location of the lattice sites is obtained by averaging \(\psi_s\) over all orientations of the symmetry axes and over all positions of the lattice within the range of a single lattice cell. This averaged wave function \(\overline{\psi}_s\) carries no information about lattice sites or symmetry axes. It retains complete information on the internal structure of the system.

A plausible general form for the exact ground-state wave function of a system of interacting bosons is

\[
\psi_0 = \Lambda_0 \exp \left[ \frac{1}{2} \sum_{i<j} U(r_{ij}) + \sum_{i<j<k} U_3(i,j,k) \right. \\
\left. + \sum_{i<j<k<l} U_4(i,j,k,l) + \cdots \right]
\]

(1)

Procedures for determining the correlation functions \(U_n(1,2,\ldots,n) \equiv U_n(r_1, r_2, \ldots, r_n)\) are described in several recent studies.\(^2\)\(^-\)\(^5\) These functions

*See Ref. 1 for a critical analysis and comparison of the published methods and numerical results for solid helium from the point of view of a highly summed diagrammatic \(t\)-matrix perturbation theory.
are taken to be invariant under permutations, rigid displacements, and rigid rotations of the coordinates. In the theory of the $^4$He system this functional form for the wave function has been considered as describing the liquid state, but there appear to be no grounds for excluding the application to describe the ground state of an unconstrained solid floating free in an inertial reference frame. We assume that the number of particles $N$ is very large, so that surface effects and the detailed mechanism by which pressure is applied to the system need not be discussed explicitly. We are interested in the possibility that $\bar{\psi}_s$ differs inappreciably from $\psi_0$ in the density range of the solid state.

Suppose that all the correlation functions $U_n$ have been determined as functions of the coordinates and of the density so that

$$E_0(v) = \min_{\Omega} \int \psi_0 H \psi_0 \, dx_1 \ldots dx_N$$

Here $v$ is the specific volume ($v = 1/\rho = \Omega/N$). In Fig. 1 the solid curve exhibits the general behavior of $E_0(v)$ required to produce a first-order phase transition.

Between $v_\alpha$ and $v_l$ the system is in the liquid phase with pressure $\geq 0$. At $v_l$ a first-order phase transition becomes possible with a liquid phase at specific volume $v_l$ and a second (presumably solid) phase at $v_s$. At specific volumes between $v_l$ and $v_s$ both phases are present in amounts determined by the conditions

$$N_s + N_l = N, \quad N_s v_s + N_l v_l = N v$$

with the solution

$$\frac{N_s}{N} = \frac{v - v_l}{v_s - v_l}, \quad \frac{N_l}{N} = \frac{v_s - v}{v_s - v_l}$$

The corresponding energy function is

$$E(v) = \frac{N_s}{N} E_0(v_s) + \frac{N_l}{N} E_0(v_l)$$

$$= \frac{v - v_l}{v_s - v_l} E_0(v_s) + \frac{v_s - v}{v_s - v_l} E_0(v_l)$$

a linear function of the overall specific volume identical with the equilibrium tangent line in Fig. 1.

In the two-phase range, $v_s < v < v_l$, it is necessary to reassess the assumption that Eq. (1) gives a plausible general form for the exact ground-state wave function. Far from being plausible, the identification of $E(v)$ [Eq. (5)] with $E_0(v)$ [Eq. (2)] seems impossible. The source of the difficulty